

Effects of magnetic anisotropy on spin dynamics of ferromagnetic frustrated chain

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Abstract. By exploiting density-matrix renormalization group techniques, we investigate the spin dynamics of a spin-1/2 one-dimensional J_1 - J_2 XXZ model with competing ferromagnetic J_1 and antiferromagnetic J_2 exchange couplings under applied magnetic fields. Numerical results of spin excitation spectra show that in the field-induced spin quadrupole regime, the longitudinal component has a gapless mode and the transverse component has a gapped mode irrespective of the exchange anisotropy. The excitation gap of the transverse spin excitation increases as the exchange anisotropy increases over the XY-like and Ising-like regions, demonstrating that two-magnon bound states are stabilized due to the easy-axis anisotropy.

1. Introduction

Frustrated quantum spin systems in low dimensions have provided a fascinating playground to explore strange new phases that have no classical analogue, and rich physics of quantum phase transitions between them. One of the simplest models with frustration and low-dimensionality is a spin-1/2 one-dimensional J_1 - J_2 Heisenberg model, in which the nearest-neighbor exchange interaction J_1 and the next-nearest-neighbor exchange interaction J_2 compete with each other. Note that when J_2 is antiferromagnetic, frustration occurs in either case of antiferromagnetic or ferromagnetic J_1 . Recent studies on the ferromagnetic J_1 case in a magnetic field have revealed that the ground state is a vector chiral (VC) state in low magnetic fields, while it turns to an exotic Tomonaga-Luttinger-liquid state in high magnetic fields [1, 2, 3, 4]. In the high-field phase, the formation of two-magnon bound states leads to a spin quadrupole state. The longitudinal spin and quadrupole correlations are quasi-long-ranged, while the transverse spin correlation is short-ranged. The so-called spin nematic (SN) state is realized in the vicinity of the saturation, while the ground state shows a crossover to a spin-density-wave (SDW) state with lowering the magnetic field. The ground-state phase diagram in the presence of the exchange anisotropy has also been analyzed numerically [5]. As for the experimental realization of the quadrupole state, LiCuVO_4 has been studied as a possible candidate material. Neutron diffraction experiments have shown that the field dependence of an incommensurate magnetic peak appearing in high magnetic fields is well explained by theoretical predictions of the quadrupole state [6]. Inelastic neutron scattering measurements have been carried out at zero magnetic field, indicating the existence of a two-spinon continuum [7], whereas the excitation spectrum in the high-field phase has not been reported yet.

To clarify the property of the field-induced quadrupole state from the viewpoint of the spin

dynamics, we have studied the dynamical spin structure factor of the spin-1/2 one-dimensional J_1 - J_2 Heisenberg model by exploiting numerical methods such as a dynamical density-matrix renormalization group [8]. In this paper, to gain further insight into the effect of the exchange anisotropy, we analyze the J_1 - J_2 XXZ model. We present numerical results on the anisotropic behavior of longitudinal and transverse spin excitation spectra, and discuss the dependence on the exchange anisotropy.

2. Model and method

We consider a spin-1/2 J_1 - J_2 XXZ model on a one-dimensional chain with N sites, described by

$$H = J_1 \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) + J_2 \sum_i (S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta S_i^z S_{i+2}^z) - h \sum_i S_i^z, \quad (1)$$

where S_i^α is the α component of the spin-1/2 operator at site i , J_1 (< 0) and J_2 (> 0) denote the ferromagnetic nearest-neighbor and the antiferromagnetic next-nearest-neighbor exchange interactions, respectively, Δ is the anisotropy of the exchange interaction, and h is the magnetic field along the z direction. In the present study, we fix $J_1 = -1$ and $J_2 = 1$, and examine the dependence on Δ .

We investigate dynamical properties by using density-matrix renormalization group (DMRG) methods in open boundary conditions [9, 10]. To clarify the characteristics of anisotropic magnetic excitations, we calculate the z and x components of the dynamical spin structure factor, given by

$$S^\alpha(q, \omega) = -\lim_{\eta \rightarrow 0} \frac{1}{\pi} \text{Im} \langle \psi_G | S_q^{\alpha\dagger} \frac{1}{\omega + E_G - H + i\eta} S_q^\alpha | \psi_G \rangle, \quad (2)$$

where $|\psi_G\rangle$ is the ground state and E_G is its eigenenergy. We set an infinitesimal value η to 0.1. The momentum representation of the spin operator in open boundary conditions is given by

$$S_q^\alpha = \sqrt{\frac{2}{N+1}} \sum_i S_i^\alpha \sin(qi). \quad (3)$$

For the calculation of the dynamical spin structure factor at a given magnetization $m = M/N$ with $M = \sum_i S_i^z$, we set the magnetic field h to be the midpoint of the magnetization plateau of m . We employ a dynamical DMRG method [10], in which we need three target states, i.e., $|\psi_G\rangle$, $S_q^\alpha |\psi_G\rangle$, and $[\omega + E_G - H + i\eta]^{-1} S_q^\alpha |\psi_G\rangle$. We perform dynamical DMRG calculations with 32 sites at $m = 0$ and $m = 0.25$ for typical values of Δ .

3. Numerical results

First, let us look at spin excitation spectra at zero magnetic field. In Fig. 1, we present intensity plots of $S^z(q, \omega)$ and $S^x(q, \omega)$ at $m = 0$. Figure 1(a) shows $S^z(q, \omega)$ at $\Delta = 1$ for the isotropic Heisenberg case, where the system is in a Haldane dimer phase [11]. Here, $S^z(q, \omega) = S^x(q, \omega)$ due to the SU(2) rotational invariance, as shown in Figs. 1(a) and 1(b). There is a sharp peak at $(q_0, \omega_0) = (16\pi/33, 0.14)$, and a large amount of spectral weight is concentrated on this peak. We note that ω_0 seems to be a finite value because of the finite-size effect. In fact, ω_0 becomes small as the system size increases, and it is extrapolated to almost zero in the thermodynamic limit. This is consistent with the renormalization group study suggesting an exponentially small gap [12]. The lower boundary of a continuum is found to form a sinusoidal dispersion, which corresponds to the des Cloiseaux-Pearson mode of spinon excitations in the limit of $J_1/J_2 = 0$, i.e., decoupled antiferromagnetic chains [13]. The sinusoidal dispersion is clearly visible due to the large intensity for $q < q_0$, while that for $q > q_0$ is less distinct, since the spectral weight is

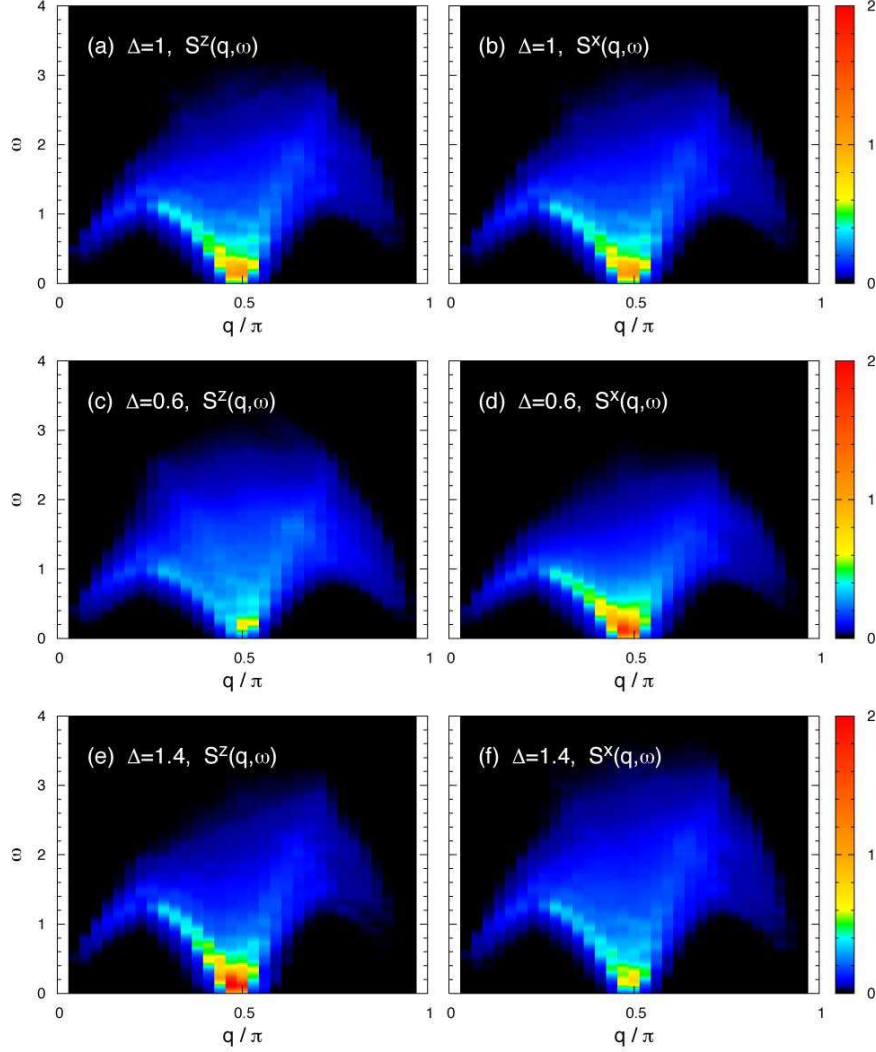


Figure 1. The dynamical spin structure factors $S^z(q, \omega)$ and $S^x(q, \omega)$ at $J_1 = -1$, $J_2 = 1$, and $m = 0$ for typical values of Δ : (a), (b) $\Delta = 1$ for the isotropic Heisenberg case; (c), (d) $\Delta = 0.6$ for the XY-like case; and (e), (f) $\Delta = 1.4$ for the Ising-like case. Three panels in the left column [(a), (c), (e)] are $S^z(q, \omega)$, and those in the right column [(b), (d), (f)] are $S^x(q, \omega)$. Here, we set $h = 0$, and the system size is $N = 32$.

distributed to a high energy region. Thus the distribution of the spectral weight is asymmetric with respect to q_0 [7, 14]. Note that the intensity extends to high energies beyond the upper boundary of the two-spinon continuum for $q > q_0$, which is indicative of a four-spinon continuum suggested in LiCuVO_4 [7].

In Figs. 1(c) and 1(d), we show $S^z(q, \omega)$ and $S^x(q, \omega)$, respectively, at $\Delta = 0.6$ for the XY-like case, where the system is in a gapless chiral phase [11]. Both $S^z(q, \omega)$ and $S^x(q, \omega)$ resemble those in the isotropic Heisenberg case in their overall spectral shapes, while they move to lower energy. We observe that the intensity at the lowest-energy peak is suppressed for $S^z(q, \omega)$, while it is enhanced for $S^x(q, \omega)$. Note that $S^z(q, \omega)$ and $S^x(q, \omega)$ have the same total intensity, and the difference of the distribution of the spectral weight in the (q, ω) space is essential. The spin excitation spectra are supposed to be gapless in the gapless chiral phase, but we do not clearly

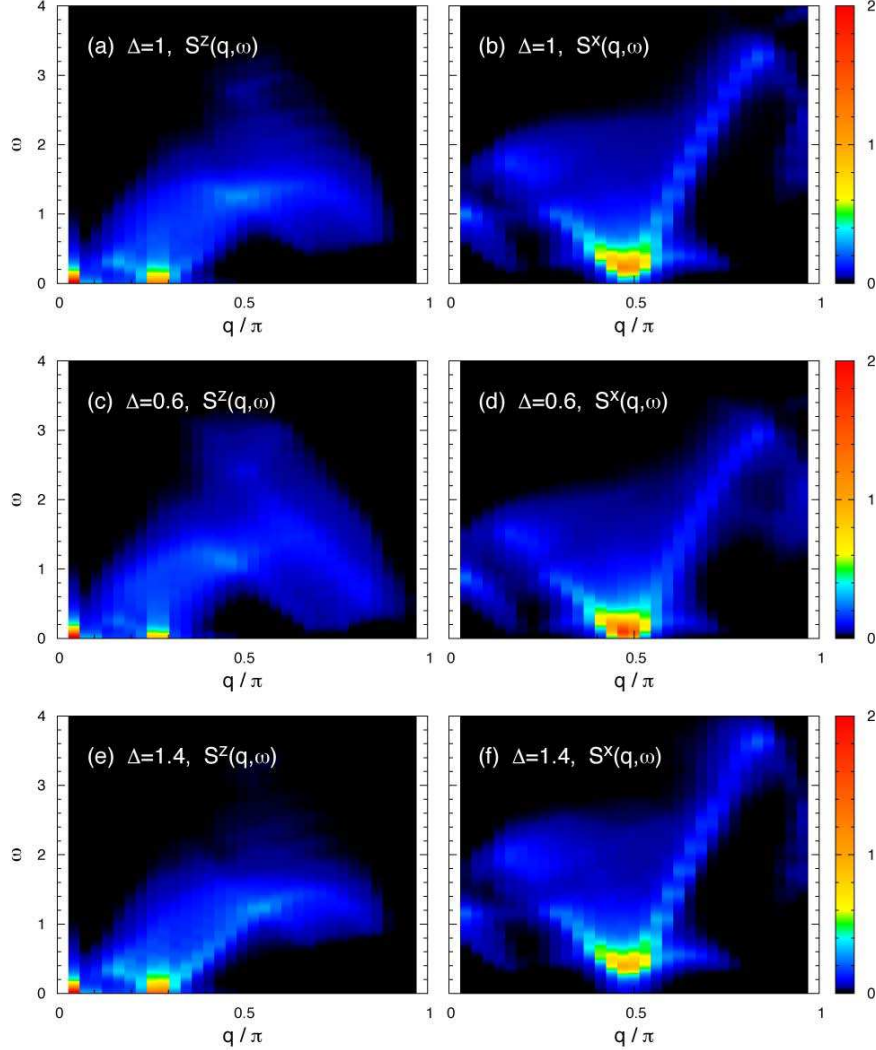


Figure 2. The dynamical spin structure factors $S^Z(q, \omega)$ and $S^X(q, \omega)$ at $J_1 = -1$, $J_2 = 1$, and $m = 0.25$ for typical values of Δ : (a),(b) $\Delta = 1$ for the isotropic Heisenberg case; (c), (d) $\Delta = 0.6$ for the XY-like case; and (e), (f) $\Delta = 1.4$ for the Ising-like case. Three panels in the left column [(a), (c), (e)] are $S^Z(q, \omega)$, and those in the right column [(b), (d), (f)] are $S^X(q, \omega)$. Here, we set $h = 1.023$ for $\Delta = 1$, $h = 0.887$ for $\Delta = 0.6$, and $h = 1.177$ for $\Delta = 1.4$, and the system size is $N = 32$.

see the gapless nature in the present results because of the finite-size effect. In Figs. 1(e) and 1(f), we show $S^Z(q, \omega)$ and $S^X(q, \omega)$, respectively, at $\Delta = 1.4$ for the Ising-like case, where the system is in the so-called uudd phase [15, 16]. The overall spectral shapes are again similar to those of the isotropic Heisenberg case, while they are pushed up to higher energy in contrast to the XY-like case. In addition, the intensity at the lowest-energy peak is enhanced for $S^Z(q, \omega)$, while it is suppressed for $S^X(q, \omega)$, which is the reverse of what we find in the XY-like case. In the uudd phase, the longitudinal spin excitation spectrum is gapless, while the transverse one is gapped, but these features are not clear because of the finite-size effect. The detailed finite-size scaling analysis is an important future problem, which will be reported elsewhere.

Now, we move on to the investigation in the magnetic field. In Fig. 2, we present intensity

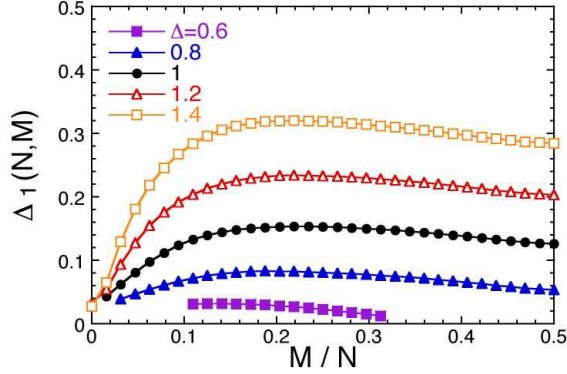


Figure 3. The spin excitation energy $\Delta_1(N, M)$ at $J_1 = -1$ and $J_2 = 1$ for several values of Δ . Here, we show the results only in the field-induced SDW/SN regime. $\Delta_1(N, M)$ in the VC phase is supposed to be zero in the thermodynamic limit. The system size is $N = 128$.

plots of $S^z(q, \omega)$ and $S^x(q, \omega)$ at $m = 0.25$, corresponding to the field-induced SDW regime. Figure 2(a) shows $S^z(q, \omega)$ at $\Delta = 1$ for the isotropic Heisenberg case. We find a lowest-energy peak at $(q_0, \omega_0) = (9\pi/33, 0.00)$. q_0 moves toward small momentum from the position at zero magnetic field. By analyzing q_0 for various values of m , we have confirmed that q_0 changes with m following a relation $q_0 = (1/2 - m)\pi$ in the field-induced SDW/SN phase [8], which supports the bosonization result [4]. On the other hand, ω_0 is nearly zero, indicating a gapless mode of the longitudinal spin excitation. Note that we also find a ferromagnetic peak at the origin due to the finite magnetization. In Fig. 2(b), we show $S^x(q, \omega)$ at $\Delta = 1$. We find a lowest-energy peak at $(q_0, \omega_0) = (16\pi/33, 0.22)$. In particular, we have verified that ω_0 is extrapolated to a finite excitation energy in the thermodynamic limit, indicating a gapped mode of the transverse spin excitation. We notice that $S^x(q, \omega) = [S^+(q, \omega) + S^-(q, \omega)]/4$, i.e., it represents the spin excitation changing the magnetization by one. Since a finite energy is required to break a bound magnon pair, we have an excitation gap corresponding to the binding energy.

All these features found in the isotropic Heisenberg case are similarly observed for both the XY-like [Figs. 2(c) and 2(d)] and Ising-like [Figs. 2(e) and 2(f)] cases. That is, for $S^z(q, \omega)$, q_0 changes with m as $q_0 = (1/2 - m)\pi$ in the field-induced SDW/SN phase, and ω_0 is nearly zero, indicating a gapless mode. For $S^x(q, \omega)$, ω_0 is found at a finite energy, while it is extrapolated to a finite excitation energy in the thermodynamic limit, indicating a gapped mode. Here, we clearly see the difference of ω_0 of $S^x(q, \omega)$ between the XY-like and Ising-like cases. Compared to the isotropic Heisenberg case [Fig. 2(b)], ω_0 decreases in the XY-like case [Fig. 2(d)], while it increases in the Ising-like case [Fig. 2(f)]. Thus the excitation gap is suppressed in the XY-like case, and it is enhanced in the Ising-like case.

To clarify the dependence of the excitation gap of the transverse spin excitation, we calculate a spin excitation energy, defined by

$$\Delta_1(N, M) = [E_0(N, M + 1) + E_0(N, M - 1) - 2E_0(N, M)]/2, \quad (4)$$

where $E_0(N, M)$ is the lowest energy of the N -site system in the subspace of M at $h = 0$. Here, we use an ordinary DMRG method, not dynamical one, to obtain $\Delta_1(N, M)$. In Fig. 3, we plot $\Delta_1(N, M)$ for several values of Δ . The results in the field-induced SDW/SN regime are shown. Note that we find reentrant behavior in the XY-like case, i.e., the ground state changes from the VC state to the SDW/SN state and turns to the VC state again as the magnetization increases from zero to the saturation [5]. We find that $\Delta_1(N, M)$ increases as Δ increases over the XY-like

and Ising-like regions. This indicates that the easy-plane anisotropy disfavors the formation of two-magnon bound states, and the easy-axis anisotropy stabilizes the two-magnon bound state, which is consistent with the behavior of correlation functions [5].

4. Summary

We have investigated the spin excitation dynamics of the spin-1/2 one-dimensional J_1 - J_2 XXZ model in the magnetic field by numerical methods. We have observed that in the field-induced SDW/SN phase, the longitudinal spin excitation is gapless, while the transverse spin excitation is gapped, irrespective of the exchange anisotropy. The excitation gap of the transverse spin excitation increases as the exchange anisotropy increases, which is indicative that the easy-axis anisotropy stabilizes the two-magnon bound state.

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